



What is NIST



NIST's primary mission is to promote economic growth by working with industry to develop and apply technology, measurements and standards.



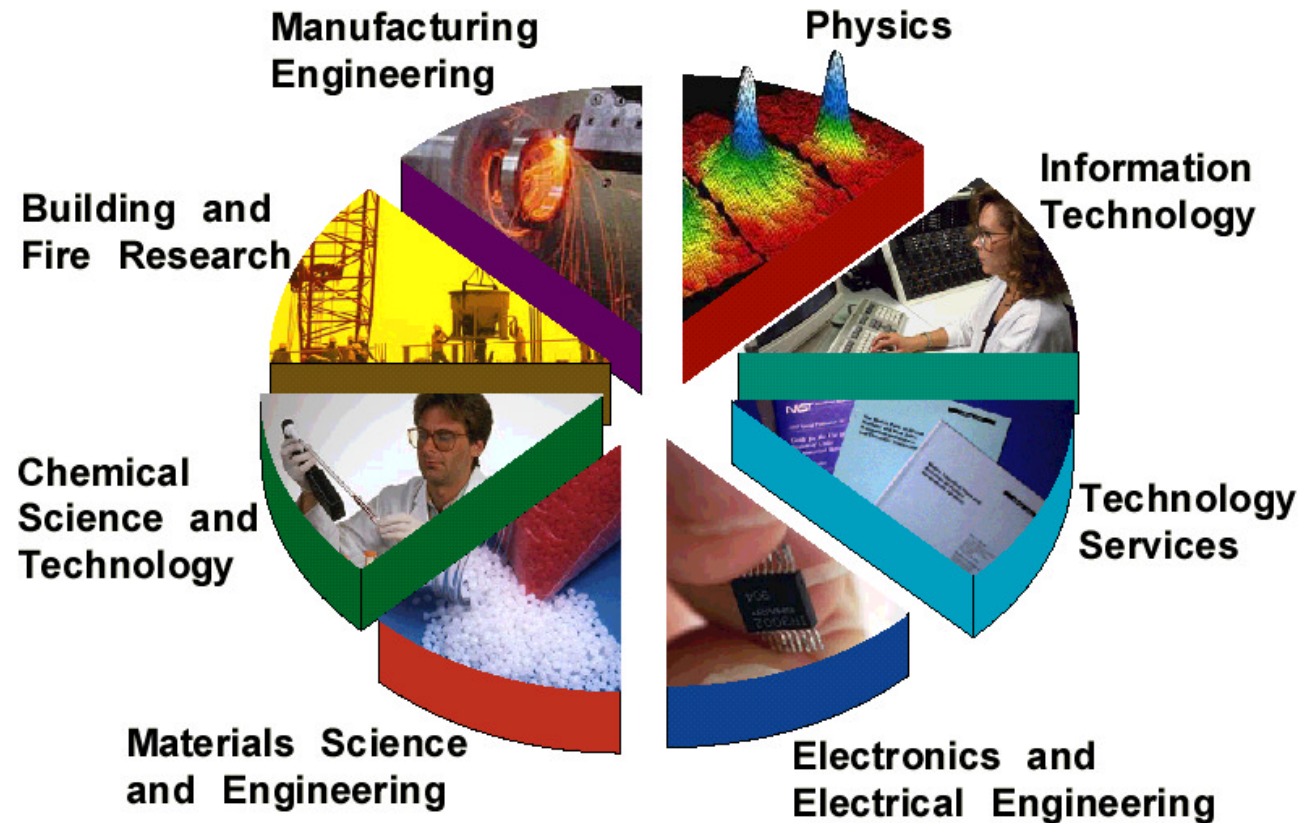
Helping America Measure Up

- NIST strengthens the U.S. economy and improves the quality of life by working with industry to develop and apply technology, measurements, and standards.
- NIST Assets:
 - 3,300 employees
 - \$800 million annual budget
 - 1,200 industrial partners
 - 2,000 field agents
 - 1,550 guest researchers
 - \$1.4 billion co-funding of industry R&D
 - National measurement standards





National Institute of Standards and Technology - Program Portfolio



Highly leveraged measurement and research capabilities supporting trillions of dollars in products and services



Why NIST?

- **Drivers for industry**

- Speed,
responsiveness,
innovation
- Reduction in time,
material, and waste
- Optimization for new
materials needs

- **Drivers for NIST**

- Rapid development of
materials data
- Validation of
combinatorial
measurements
- Connections to
fundamental science



Agenda for Today's Workshop

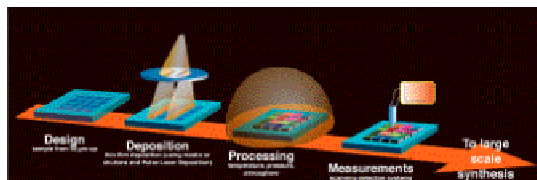


AGENDA FOR NIST COMBINATORIAL METHODS CENTER KICK-OFF MEETING, JANUARY 23, 2002, SAN DIEGO

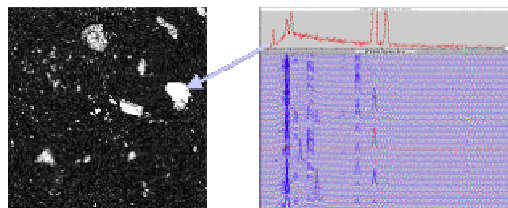
- 7:30 Registration and Coffee
- 8:30 *Welcome and Introductions – Eric Amis*
- 8:50 *Combinatorial Adhesion – Alfred Crosby*
- 9:10 *Multispectral Imaging for Materials Analysis – Steven Buntin*
- 9:30 *High-throughput Transport and Diffusion - Chris Muzny*
- 9:50 *Multiscale Patterned Biosurfaces – Eric Amis*
- 10:10 Coffee Break
- 10:30 *Combinatorial Tools for Inorganic Materials – Debra Kaiser*
- 10:50 *Polymer Formulations – Alamgir Karim*
- 11:10 *High-throughput Flame Retardants – Jeffrey Gilman*
- 11:30 *Combinatorial Polymer Crystallization – Kathryn Beers*
- 11:50 *Other Current Topics –Alamgir Karim*
- 12:10 Lunch
- 1:15 *Center Organization (Projects, Costs, Benefits) –Eric Amis*
 Participating Membership Level
 Focused Projects
 CRADA's



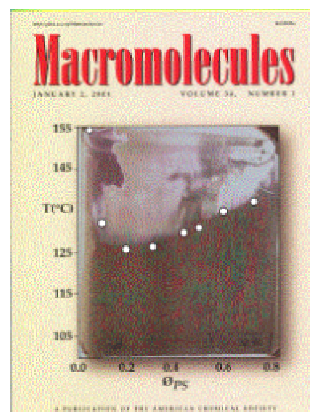
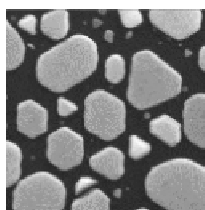
Combinatorial Methods at NIST



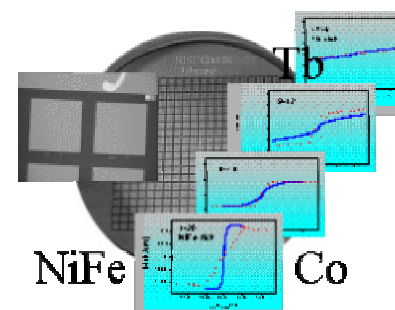
Polymers
 Polymer blend phase behavior
 Biocompatibility assay
 Adhesives
 Surface chemistry and modification
 Semi-crystalline polymers
 Block-copolymer ordering behavior
 Fire retardants
 Library production support
 Laser scanning microscopy



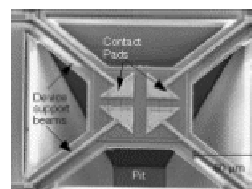
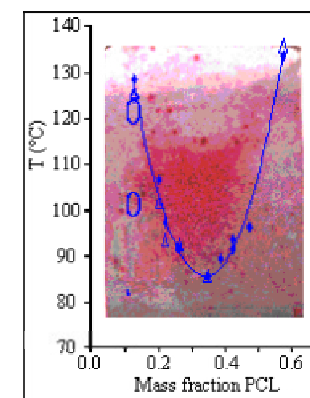
Chemical Analysis
 Chemical microscopy by SIMS
 Data mining: Searching for patterns
 Quantitative spectral imaging
 Infrared chemical imaging



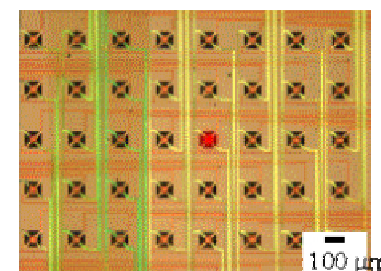
Metals and alloys
 Dielectric oxide thin films
 Metallization of GaN semiconductors
 TEM studies of combinatorial libraries
 Polarized light scattering



Biomaterials
 Biocompatibility assay
 Surface Hydrophobicity
 Bio-adhesion
 Cell growth and differentiation
 Patterned cellular activity



Thermal Properties
 Service life prediction
 Microhotplate array platforms
 Modeling and characterization





Assessing Needs and Initiation

Visitors to NIST Combi labs

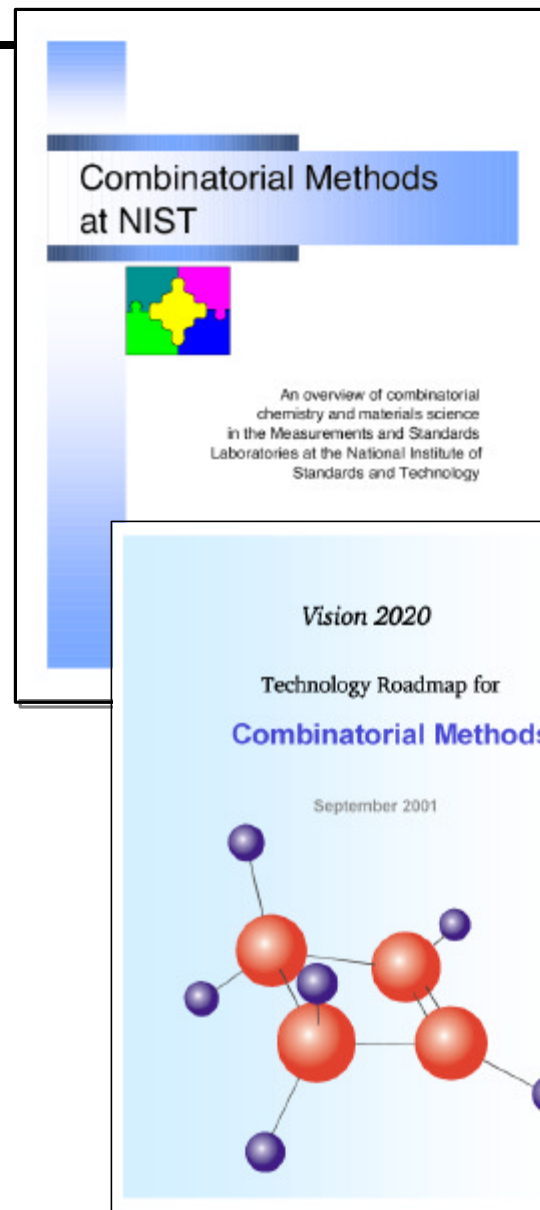
Air Products, Army Research Lab, Asahi Chemical, BASF, Bayer, Dow Chemical, Dow Corning, ExxonMobil, GE, Pall Corporation, Rhodia, Rohm & Haas, TotalFinaElf, Wright-Patterson

Key Findings from NIST Vision 2020 Workshop

- US industry slow to adopt “combi” compared to Europe
- No coordination for industry/government/academia to collaborate
- Combi must be extended to more complex systems
- Cost of combi must be reduced
- *Priority for NIST to facilitate methodology and standards*

Leadership roles for NIST labs

- Symposium on “Combinatorial and Artificial Intelligence Methods in Materials Science” for Fall 2001 Materials Research Society National Meeting (69 papers over 3.5 days)
- Special focus issue on “Combinatorial and High-Throughput Methods for Materials Science” as the April 2002 issue of the *Bulletin of the Materials Research Society*
- Founding of new Gordon Research Conference on “Combinatorial and High-Throughput Methods for Materials Science” to be held June 30-July 4, 2002
- Several edited monographs and encyclopedia entries in preparation to collect insights from early adopters





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Participating Membership Level
Focused Projects
CRADA's

Materials Science and Engineering Laboratory

Polymers Division

Home Research Areas

The NIST Combinatorial Materials Center
Describes the Center's objectives, structure, and activities.

Kick-Off Meeting in San Diego
Register Now! In conjunction with Combimaterials 2002.

Calendar of Events
List of recent events at the Center include Future Meeting Dates: July 2001, December 2001, and February 2002.

What's New at the NCMC
List of recent projects and news at the Center.

Combinatorial and High-Throughput
NIST Combinatorial and high-throughput materials research.

CRADA Projects
Information regarding Cooperative Research and Development Agreements.

Publications
PDF files of papers, reports, and preprints.

Bulletin Board
Comments and replies on combinatorial materials research.

Library Preparation and Characterization
Brief description of sample preparation, throughput research.

Data Libraries
Select data libraries available for viewing.

For further information send e-mail to Alfred.Lewis@nist.gov

NIST Material Science & Engineering Laboratory



COMBI 2002

COMBINATORIAL APPROACHES FOR NEW MATERIALS DISCOVERY

4th Annual International Symposium on

January 23-25, 2002 • Four Points Sheraton Hotel • San Diego, CA USA

In it's 4th biennial meeting year, Combi 2002 meets the demands of industry, government and academia by addressing numerous technology transfer issues which are essential to transition technology to the marketplace. The meeting will examine the latest developments in:

- COMBINATORIAL AND HIGH THROUGHPUT METHODS**
 - High throughput technology: recent advances and new ideas
 - Achieving "production mode" status in a high throughput experimental set-up
 - Technology scale-up
- EXPERIMENTAL DESIGN FOR PARALLEL LIBRARIES AND HIGH THROUGHPUT SCREENING**
 - Analysis of combinatorial and high throughput characterization of combinatorial materials libraries
 - Designing the experiment for combinatorial materials discovery
 - Developing instrumentation and solutions for implementing high throughput workflows
- SYNTHESIS AND DISCOVERY OF NEW MATERIALS:**
 - Combinatorial manufacturing of organic, inorganic, and hybrid materials
 - Combinatorial methods for organic and polymeric materials
 - Combinatorial tools for inorganic and heterogeneous catalysis
 - Combinatorial approaches to nanoscale and photonic materials
- MULTIVARIANT MEASUREMENTS**
- METROLOGY, INSTRUMENTATION AND TOOLS FOR COMBI**
- HIGH THROUGHPUT EXPERIMENTATION INFORMATICS AND DATA PROCESSING**
- FEATURED PANEL DISCUSSION ON MAKING COMBI THE SAME EFFICIENT INSTRUMENT IN MATERIALS SCIENCE AS IT IS IN DRUG DISCOVERY**

SPECIAL PRE-CONFERENCE WORKSHOP
COMBI & HIGH THROUGHPUT SYNTHESIS: TECHNOLOGY TRANSFER, MARKET CHALLENGES & INVESTMENT PROSPECTS

The National Institute of Standards and Technology presents
THE ESTABLISHMENT OF THE COMBINATORIAL MATERIALS CENTER AT THE NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
Wednesday, January 23, 2002 12 noon (Poker Room 446B) • San Diego, CA
12:00pm - 2:00pm

Continuously Updated

NIST

The National Institute of Standards and Technology presents
**THE ESTABLISHMENT OF THE COMBINATORIAL METHODS CENTER AT
 THE NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY**
Wednesday, January 23, 2002 • Four Points Sheraton Hotel • San Diego, CA
7:30am - 2:30pm

Conveniently Timed

Prior to the Knowledge Foundation's COMBI 2002 Symposium, the National Institute of Standards and Technology (NIST) will hold a meeting to present and discuss establishment of a Combinatorial Methods Center at NIST.

Talks will be presented by NIST researchers and invited speakers.

Morning session will feature presentations on measurement science challenges posed by Combinatorial Materials Research.

This meeting is presented for the convenience of the participants. NIST does not endorse any commercial products.

Afternoon session will provide an exciting snapshot of new research opportunities at NIST's Combinatorial Methods Center.

Scientists from different research areas of NIST will be available to discuss focused research topics and potential collaborations with the NIST Combinatorial Methods Center.

For a complete, detail agenda of this seminar please visit www.knowledgefoundation.com under COMBI 2002 or www.nist.gov/combi.

Participants, NIST does not endorse any commercial products.

Participating Membership

Focused Projects

Partnerships

[illegible]



NIST Combinatorial Methods Center, NCCMC

NCCMC Objectives

Promote dissemination of
information on combinatorial
measurement methods

Provide coordinated outreach for
NIST-MSL research activities that
support combinatorial methods

Participating
Membership

Focused
Projects

Partner
Memberships

Industry

Academia

National
Laboratories

An administrative portal for industrial interactions



NIST Combinatorial Methods Center, NCMC

Promote dissemination of information on combinatorial measurement methods for materials science between industry, university, and national laboratories

- **Participating Membership**

- Technical meetings presenting work on combinatorial methods from NIST, industry, and others
- Members short courses, workshops, demonstrations
- Members web-site for bulletin board, preprint service, speakers list, etc.

- **Focused Projects**

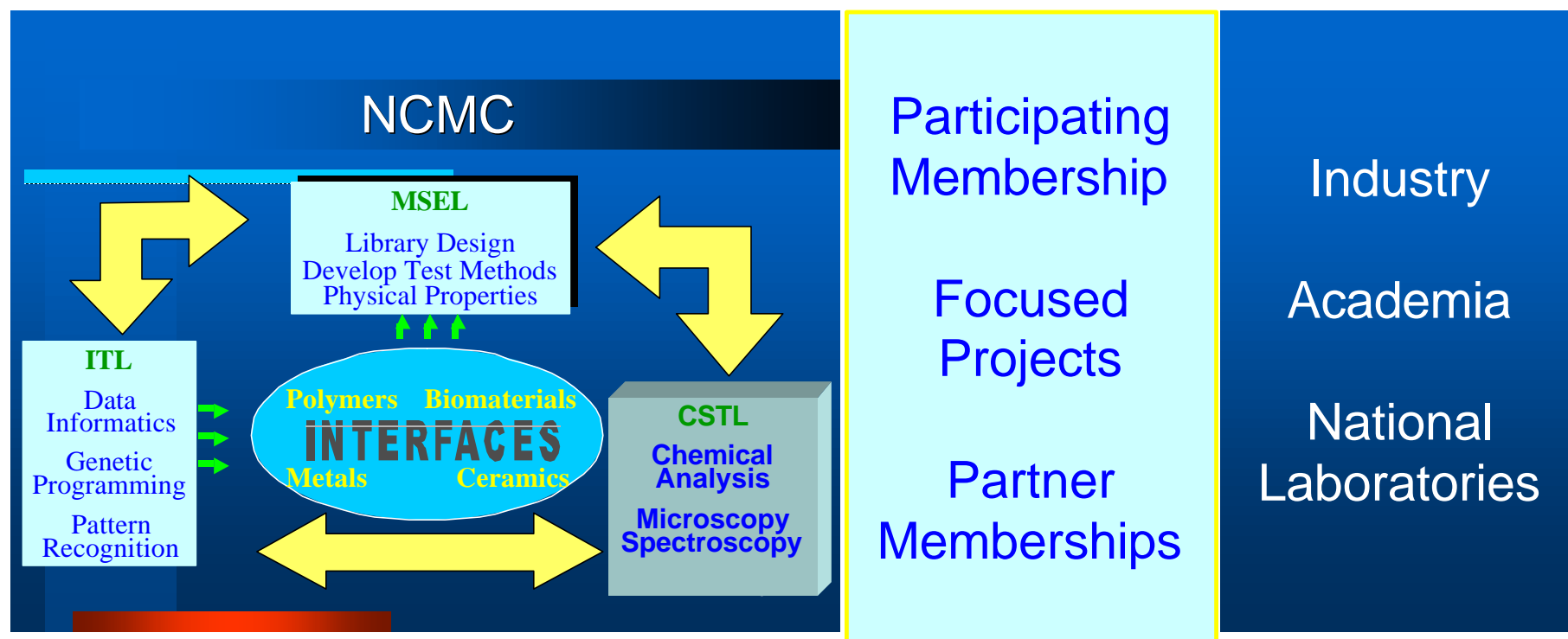
- Non-proprietary projects on new methods and applications in areas of interest to participants
- Topics chosen by member companies in cooperation with NIST technical teams
- Closed semi-annual meetings; No proprietary information disclosure; All research results publishable
- Administrative support from NCMS

- **Partner memberships**

- CRADA's partnerships with individual member organizations
- Develop methodology and applications to problems of mutual interest
- Projects may involve proprietary information and materials under I.P. agreements
- Coordination support from NCMS



NIST Combinatorial Methods Center, NCCMC



Building a research project around a technical issue



NCMC Participating Membership

Description: Members will be invited to attend semiannual technical meetings where combinatorial research on materials science will be presented.

Quarterly, members-only meetings will provide focused short courses, workshops or demonstrations.

Members will have access to a web-site for bulletin board, preprints, and speakers information.

Membership is for one year, renewable on a yearly basis.

New members may join at any time.

No proprietary information will be disclosed.

The NCMC will provide administrative support for organization of the meetings and Member services.

Member fees: \$10,000 U.S. per Member per year. NIST reserves the right to lower this fee.



NCMC Focused Projects

Description: Members will develop combinatorial projects in areas of joint interest coordinated by NIST technical teams.

Projects will not involve any proprietary information or materials and all results will be publishable.

The NCMC will provide administrative support for projects. Membership is for one year at a time, renewable on a yearly basis.

There is no restriction on the number of projects that a Member may join or when Members may join any project(s).

Each project will be for one year, renewable for additional years.

Closed semi-annual meetings held in conjunction with the Participating membership semi-annual meetings to discuss progress on projects.

Additional meetings can be scheduled by NIST technical teams.

Participating membership is required.

Member fees: To be decided by project team.



NCMC Partner Memberships

Description: CRADA partnerships with individual member organizations will be established.

The purpose is to develop combinatorial methodology and materials properties measurement techniques and apply to materials science problems of mutual interest.

Projects may involve proprietary information and materials under intellectual property (I.P.) agreements.

The coordination of the CRADA and administrative support will be provided by NCMC.

Each CRADA project will be subject to a separate agreement regarding Statement of Work (SoW), fees (if any), proprietary information and I.P. rights. Participating membership is required.

Member fees: To be decided by individual CRADA team.



NCMC Workshops and Outputs

Participating Members

- Technical workshops with NIST updates and new directions
- Reviews of current advances elsewhere, external speakers and literature reviews
- Member input for future directions and needs assessment
- Hands-on laboratory demonstrations and testing

Example: Library preparation

Details of preparation methods
Designing variations in parameters
Successes and failures
Constraints
Automations

In the future: Adhesion, Robotics and Programming,
Informatics, Data Standards, Optical Properties,
Electric Properties, Mechanical Property Tests,
Bio-Responses, Solutions/Suspensions, Ink-Jetting,
Spectral Imaging, Visualization of Data/Information

Variations: Composition
Thickness
Temperature
Surface energy
Crosslinking
Roughness
Phase separation
Domain size
Crystallinity
Additives
Reactivity rates

Focused Projects

- Specific topic meetings with project members for direction and reporting

Non-Travel Mechanisms for participation and dissemination



NCMC - Internal Issues

Provide coordinated outreach for NIST Labs research activities using and supporting combinatorial methods for chemistry and materials science

- **Participating Membership**

- Fee pays for administrative support to organize meetings, provide web site, make connections between NIST researchers and potential customers, prepare and distribute informational materials.
- Charging a fee produces a measure of “buy-in” from industry or other partners, assures that someone at the company will have and take responsibility for coordinating interactions with appropriate people inside the company even as these people change.
- “Membership” also brings the activity to a higher level of recognition within the company
- The level of buy-in should also increase credibility of effort within NIST

- **Focused Projects**

- These projects could be very similar to many current research collaborations
- Within the center there would be a standard agreement with few options (fee, in-kind, period of performance, participants, statement of work). This should greatly reduce the burden of setting up these agreements by removing many items from the table.
- By keeping the work non-proprietary we can include universities as partners, and we can include guest researchers on the project team.
- By keeping the work publishable we are more likely to meet the standards of pre-competitive and broadly applicable research. This will also help us attract good scientist to work on the projects.
- In addition to providing administrative support to these projects, being associated with the center should provide synergies as part of a bigger activity.



NCMC - Internal Issues

Partner memberships

- CRADA's can be established much as is currently done
- Most are with individual companies
- If we can provide a framework agreement it may help facilitate and it could provide a standard solution for the relationship with other center activities
- For multi-company agreements it might be best to have a standard initial agreement
- Coordination support could be provided

Example issues and straw men

- Center membership \$10K (associate membership at lower level for small companies who would like to provide research support)
- Focused projects could charge fees as the participating OU's choose or not charge at all
- Depending on the level of support from the center focused projects could contribute a modest amount. (The benefits of this charge mirror the benefits described for external.)
- Potential focused project topics: flame retardants, adhesion measurements, nucleation in polyolefins, ink jet library preparation, fillers effects on polymer blends
- Potential workshop topics: ink jet library preparation, spectral imaging, thermal measurements, connections to pharma, data management strategies, data visualization



Early Work on the Grand Canyon

